The effect of thermal fluctuation on impacts of nanoclusters

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The effect of thermal fluctuation on impacts of nanoclusters

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少数の原子から成る3次元のナノクラスターモデルを構成し、クラスター衝突の分子動力学シミュレーションを行った。温度一定の平衡状態におかれた2個のクラスター同士を、熱速度よりも小さい相対速度で正面衝突させると、衝突速度と反発係数の関係はマクロな物質が示す1/5乗則に従うことがわかった。また、衝突速度が低速の領域においては、反発係数は熱揺らぎの効果によって1以上の値を取り得ることもあることがわかった。更にクラスター同士を低速で正面衝突させたときの反発係数の出現確率の分布と、衝突を時間反転させて計測した反発係数の出現確率の分布から、衝突問題における揺らぎの定理との比較を行なった。

Recently, theorists have developed several theoretical results known as the fluctuation theorem (FT), which has been numerically and experimentally tested.[1] FT estimates the probability of emergence of the negative entropy production in tiny objects subject to large thermal fluctuation.

We have performed a molecular dynamics simulation of collision of nanoclusters and investigated the relation between FT and impact phenomena of argon clusters. We have arranged two identical nanoclusters, each of which is consisted of 682 argon atoms governed by the Lennard-Jones potential(Fig. 1). Initially, the configuration of atoms of a cluster has a FCC structure. We define the initial temperature of the clusters by the variance of the normal distribution for the initial velocities of atoms. After equilibrating the clusters to an arbitrary temperature, we have made the two clusters collide head-on with the initial velocities smaller than the thermal velocity of the system. We assume the interaction between the two clusters as the repulsive part of the Lennard-Jones potential. By changing the set of initial velocities of all the atoms and the initial orientation of the cluster, we have carried out 1000 simulations per initial condition and averaged the results.

From our simulation, it became clear that the relation between the relative colliding speed v and the restitution coefficient e obeys $a - e \propto v^{1/5}$, where a is a parameter larger than unity when the initial temperature ranges from $T = 0.01E/k_B$ to $T = 0.03E/k_B$. Here, E and k_B are

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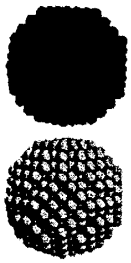

図 1: Numerical model of nanoclusters. Each of them is composed of 682 atoms which are bound together by the Lennard-Jones potential.

the scaling unit of energy and the Boltzmann constant, respectively. When a is equal to 1, this relation becomes the quasistatic theory of low-speed impact of elastic materials.[2] In addition, it became clear that the frequency distribution of the restitution coefficient has the Gaussian form when $v = 0.02\sqrt{E/m}$, where m is the mass of an atom.

We also have investigated the relation between our numerical results and FT for impact problems. In order to do that, at first, we have obtained the probability function of e, $P(\epsilon)$, where $\epsilon = 1 - e^2$. After equilibrating the rebounded clusters, we made the clusters collide again with the rebounded speed to measure the restitution coefficient of the time reversal trajectory, $\bar{e}$, and obtained the probability distribution $\bar{P}(\bar{\epsilon})$, where $\bar{\epsilon} = 1 - \bar{e}^2$. According to FT for impact problems, the connection between P and $\bar{P}$ becomes

$$\exp(\beta W)P(\epsilon) = \bar{P}(\bar{\epsilon}), \tag{1}$$

where β is the inverse temperature and W is the energy loss of the center of mass. In our simulation, when the initial temperature is $T = 0.02E/k_B$, it became clear that the connection between $P(\epsilon)$ and $\bar{P}(\bar{\epsilon})$ shows a good agreement with the above expression.

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